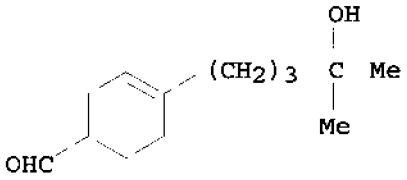
L18 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 31906-04-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Cyclohexene-1-carboxaldehyde, 4-(4-hydroxy-4-methylpentyl)- (CA INDEX NAME)
OTHER NAMES:
CN 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexene-1-carboxaldehyde
CN 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexenecarboxaldehyde
CN 4-(4-Methyl-4-hydroxyamyl)cyclohex-3-ene carboxaldehyde
CN Liral
DR 56493-02-8, 80449-98-5
MF C13 H22 O2
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM, CSNB, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, PROMT, RTECS*, SCISEARCH, TOXCENTER, USPAT2, USPATFULL, USPATOLD
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

171 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
172 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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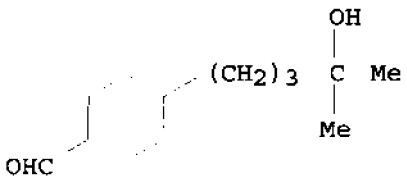
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.2	1



Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Boiling Point (BP)	120 deg C	Press: 1 Torr	(1) CAS
Density (DEN)	0.9941 g/cm**3		(1) CAS
Refractive Index (RI)	1.4915	Temp: 20 deg C Wavlen: 589.3 nm	(1) CAS

(1) Teegarden, Robert W.; US 2947780 1960 CAPLUS

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE

Bioconc. Factor (BCF)	49.44	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 10 25 deg C	(1)
Boiling Point (BP)	318.7+/-42.0 deg C	760 Torr	(1)
Density (DEN)	1.023+/-0.06 g/cm**3	20 deg C 760 Torr	(1)
Enthalpy of Vap. (HVAP)	64.94+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	135.1+/-20.5 deg C		(1)
Freely Rotatable Bonds (FRB)	6		(1)
H acceptors (HAC)	2		(1)
H donors (HD)	1		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	3		(1)
Koc (KOC)	567.49	pH 1 25 deg C	(1)
Koc (KOC)	567.49	pH 2 25 deg C	(1)
Koc (KOC)	567.49	pH 3 25 deg C	(1)
Koc (KOC)	567.49	pH 4 25 deg C	(1)
Koc (KOC)	567.49	pH 5 25 deg C	(1)
Koc (KOC)	567.49	pH 6 25 deg C	(1)
Koc (KOC)	567.49	pH 7 25 deg C	(1)
Koc (KOC)	567.49	pH 8 25 deg C	(1)
Koc (KOC)	567.49	pH 9 25 deg C	(1)
Koc (KOC)	567.49	pH 10 25 deg C	(1)
LOGD (LOGD)	2.53	pH 1 25 deg C	(1)
LOGD (LOGD)	2.53	pH 2 25 deg C	(1)
LOGD (LOGD)	2.53	pH 3 25 deg C	(1)
LOGD (LOGD)	2.53	pH 4 25 deg C	(1)
LOGD (LOGD)	2.53	pH 5 25 deg C	(1)
LOGD (LOGD)	2.53	pH 6 25 deg C	(1)
LOGD (LOGD)	2.53	pH 7 25 deg C	(1)
LOGD (LOGD)	2.53	pH 8 25 deg C	(1)
LOGD (LOGD)	2.53	pH 9 25 deg C	(1)
LOGD (LOGD)	2.53	pH 10 25 deg C	(1)
LOGP (LOGP)	2.532+/-0.257	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.63 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	Unbuffered Water pH 7.00 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.0030 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 5 25 deg C	(1)

Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	Unbuffered Water pH 7.00 25 deg C	(1)
Molar Volume (MVOL)	205.4+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	210.31		(1)
PKA (PKA)	15.31+/-0.29	Most Acidic 25 deg C	(1)
Polar Surface Area (PSA)	37.30 A**2		(1)
Vapor Pressure (VP)	2.94E-05 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2008 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

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